
Challenges in the Evaluations of Fission Data

Resolving Discrepancies, Using Fundamental & Integral Data

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Overview:

Challenges we face in evaluation

Three examples : FPY, PFNS, fission cross sections

Key Messages

- **Advancing our fission understanding, as embodied in ENDF files, will require integrated efforts in theory, experiment, & simulation**
- **Small scale science & integral measurements both essential**
- **Our progress is slow**
 - Difficult problems take a long time to solve
 - Even when they're ``solved'' we must corroborate our findings

Challenges in Creating Evaluated Data Files, Based on Experiment, Theory, Statistical Analyses & Integral Data

- **We endeavor to represent the reactions in the most accurate way possible – both physical fidelity, and numerical fidelity & completeness**
- **Experiments often discrepant. Evaluations are are best estimates with credible covariances**
- **Often much data already exists**
 - How to best incorporate new information from latest “best ever” experiments, with supposedly smaller (& different) systematical errors [TPC, Chi-nu experiments]
- **How to incorporate integral information ?**
 - K-eff criticality
 - Semi-integral
 - reaction rates (cross sections in broad sources)
 - transmission data

ENDF files serve many purposes

- **Most accurate understanding of certain reactions, cross sections**
 - Standards (IAEA, NEA, ENDF)
 - Repository for our advancing knowledge – *stewarded by DOE/Science*

- **Usage in nuclear technologies, where predicting certain integral quantities accurately is essential**
 - Transport
 - Criticality *Significant \$ in this (\$B) DOE/*
 - Energy deposition *NNSA, NE,*
 - Activation
 - ...

It is a challenge to satisfy all these goals, given our incomplete knowledge & understanding, & the range of our “customers”

This can lead to religious wars between two factions

- **One extreme: The fundamental-science fundamentalists**
 - Respect only differential measurements
 - Abhor integral data, and usually don't understand the applications
 - Perfectly happy to get the wrong integral answers for the right reasons

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 - Understand the mission imperative to get the right answer for integral problems
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ENDF/B-VII strives for good judgment in seeking the middle ground:

- more rigorous and defensible, using many advances in physics, methods
- but judicious (even ad-hoc) "tweaks" made for integral performance
- created trust with our users, cited >4000 times

And By The Way, This Issue is Everywhere

- **Material science**
 - metallurgy “heat and beat”



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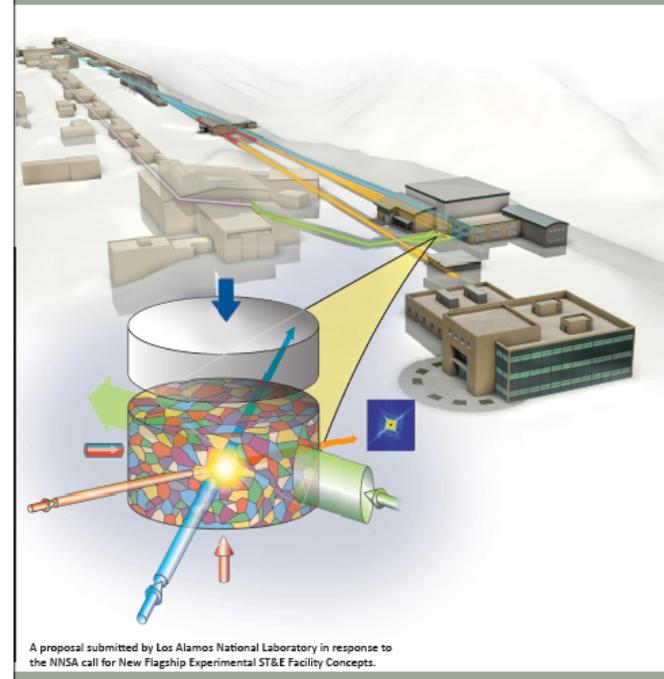
- **Material science**

- metallurgy “heat and beat”



- v. fundamental physics “micron gap” MaRIE
– Los Alamos’ vision for a future flagship facility

MaRIE 1.0: A Flagship Facility for Predicting and Controlling Materials in Dynamic Extremes



Los Alamos’ history is of solving challenging multi-physics problems using both approaches synergistically

Example 1: Fission Product Yield (FPY) Evaluations to Resolve a Longstanding LANL-LLNL Discrepancy

The issue

- Los Alamos & Livermore were discrepant on their views of the ^{239}Pu ^{147}Nd FPY
- Led to an offset in the “fission basis”

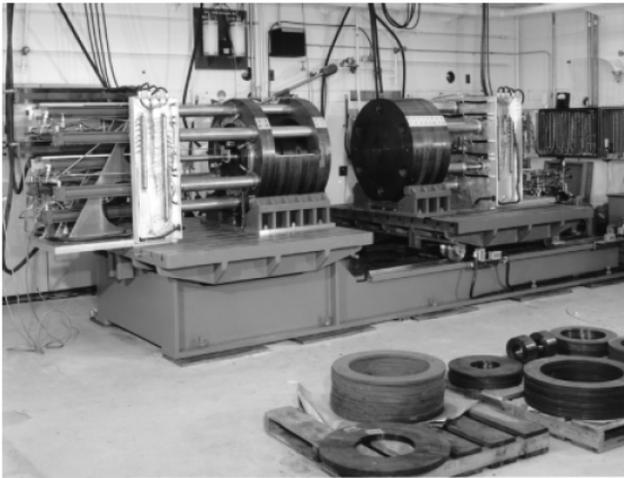
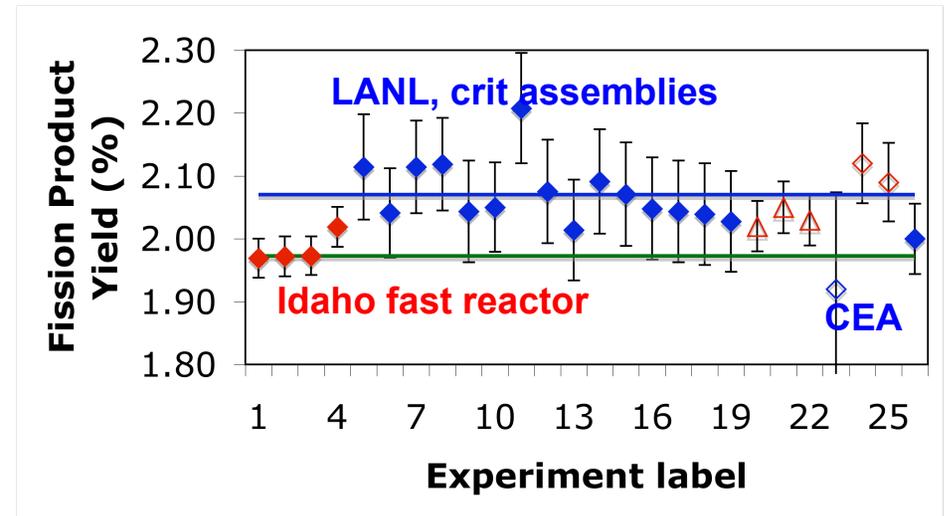


Figure 1. The Big Ten Assembly during Construction (1968).

147Nd FPY Data set seemed to exhibit discrepant data (~10% spread):

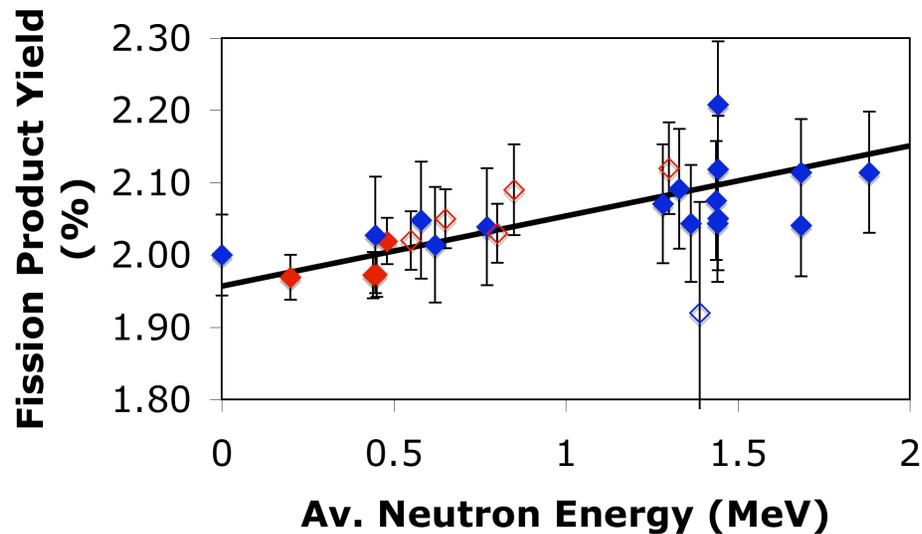


Goal: Resolve discrepancies & seek understanding @ ~ 2% level

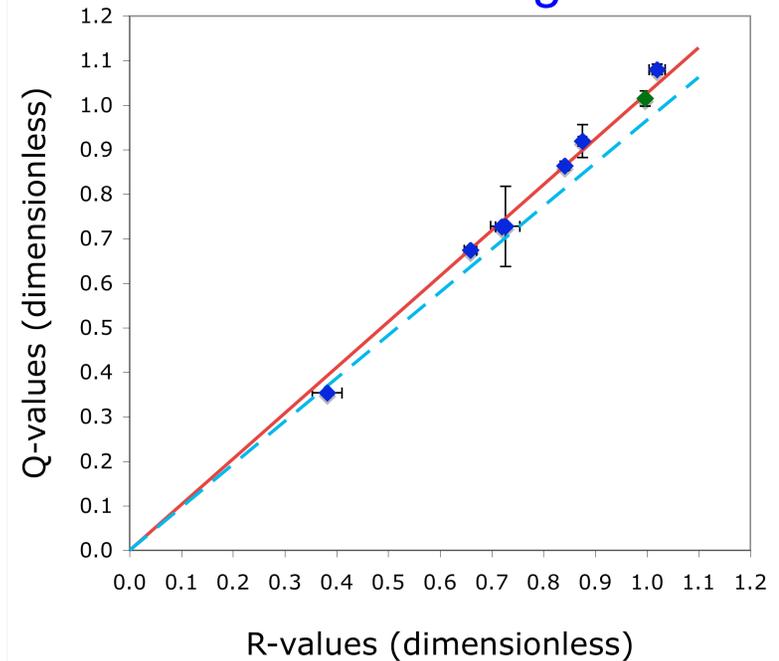
Evaluation Work Looks for Patterns..

Allowed us to Determine the ^{147}Nd FPY to $\sim 2\%$ @ 1.5 MeV

Identification of an energy-dependence



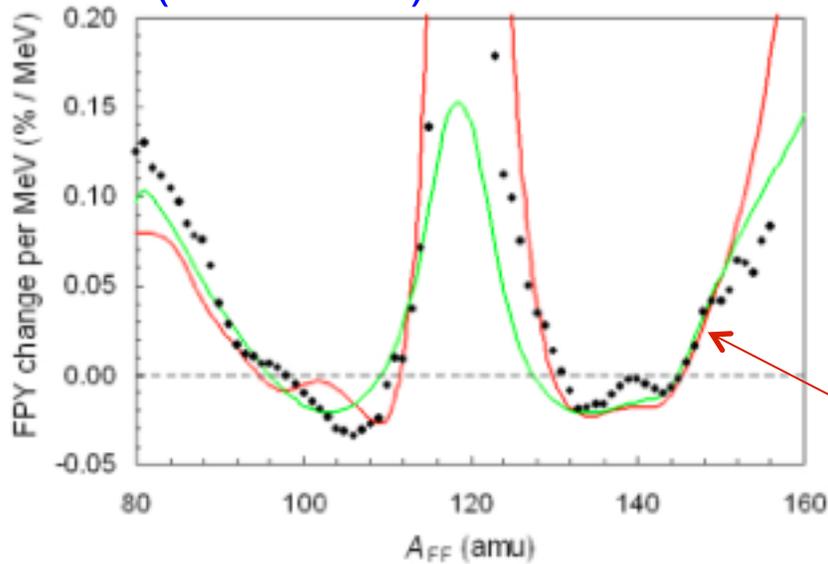
A statistical meta-analysis supported our LANL understanding



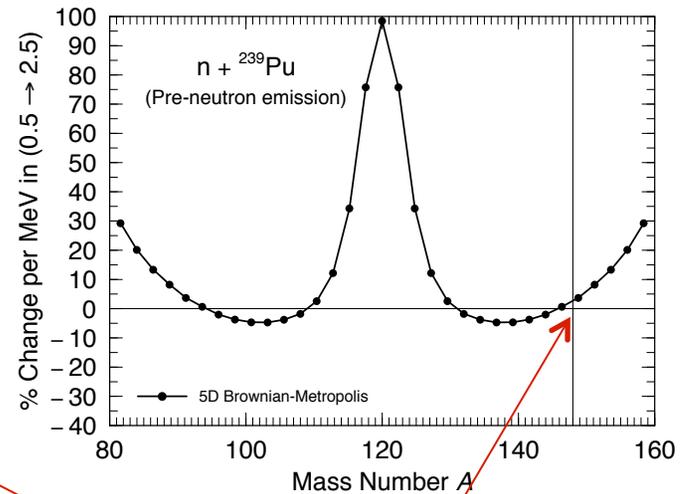
Next steps: corroborate our understanding with experiments & initiate a theory effort to understand FPY energy dependencies (see talks from Lestone, Sierk, Moller, & Younes work)

Theory progress on broader understanding of trends of FPY energy-dependencies in fast range

Lestone predictions (black points) compared with our ENDF/B-VII.1 trends (color lines)



New Moller predictions



147Nd FPY has slightly positive energy trend

FIG. 29: The relative percentage changes in the $n + {}^{239}\text{Pu}$ FPY per MeV increase in the energy of the incident neutron versus the fission-fragment mass number. The solid-black circles show our calculated relative yield changes from $E_n=0$ to 2 MeV. The green curve shows the relative changes between broadened ENDF/B-VII.1 FPY at $E_n=0.5$ and 2.0 MeV. The red curve shows the relative changes per MeV between the $E_n=0$ and 2.0 MeV ENDF/B-VII.1 evaluations.

Follow- on Experiments from TUNL-LANL-LLNL Team

Progress

- Probably best-ever activation measurements now made, at various mono-energetic energies (see Gooden, Tonchev talks)
- Corroborate our understanding at fission spectrum energies
- But raised new questions
 - But raised more questions, e.g. 14 MeV
 - Energy dependencies as a func. of A

New TUNL data support our predictions for ^{147}Nd

(see Gooden, Tonchev, Vieira, Wilhelmy, et a.)



Next steps, to help resolve these questions...

SPIDER detector measurements (Toveson)

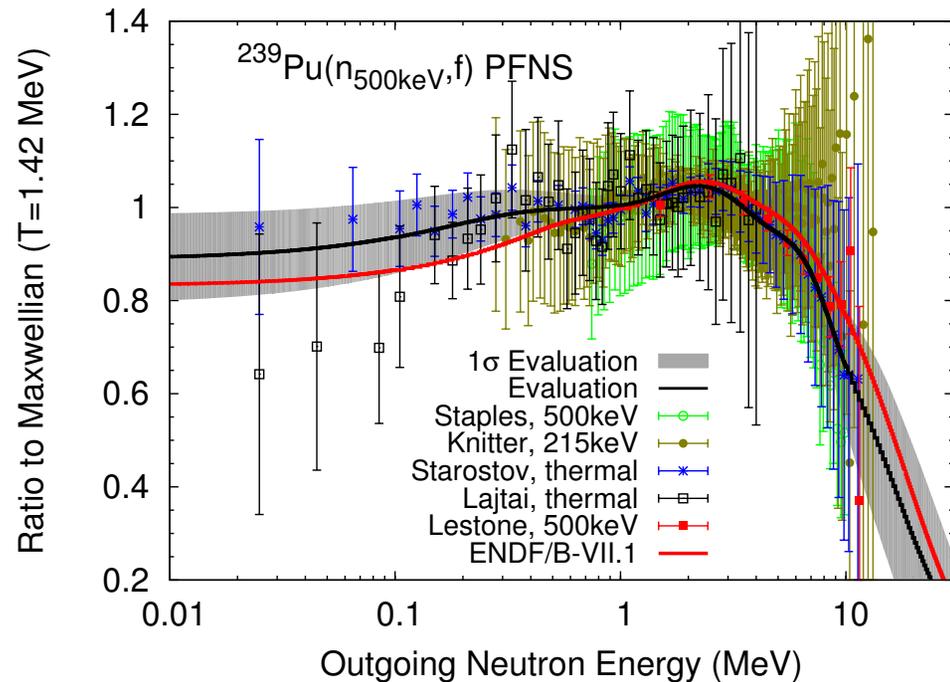
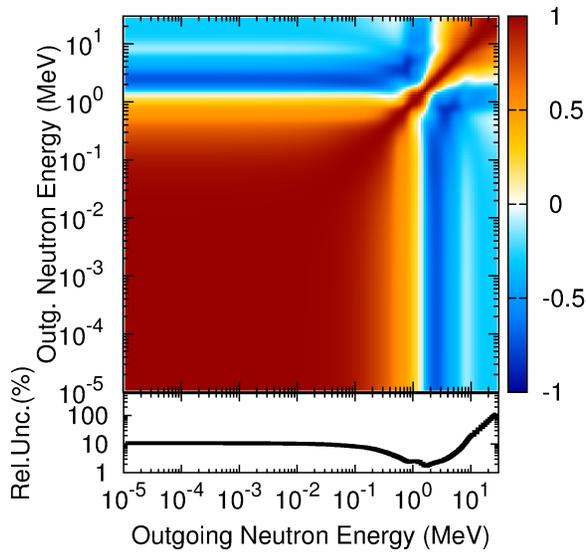
Example 2: Prompt Fission Neutron Spectrum....

- **Theory and experiment are both essential**
- **Both face challenges**
 - Theory predictive power is weak – different assumptions give vastly different predictions
 - Experiments suffer from a wide range of systematic error (data are all over the map)
 -

Prompt Fission Neutron Spectrum $n(0.5 \text{ MeV})+^{239}\text{Pu}$ - With International Collaboration Via an IAEA CRP

Recent evaluations from T-Division based on:

- Extended Los Alamos model (anisotropy, different temperatures in light and heavy fragments, etc.)
- Extensive analysis of past and present experimental data and setups
- Use of NUEX data
- Generalized least-square



Extend up to 30 MeV

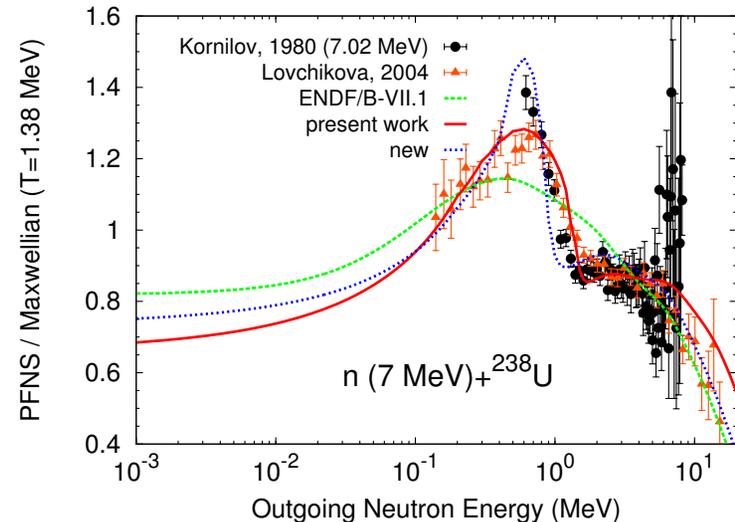
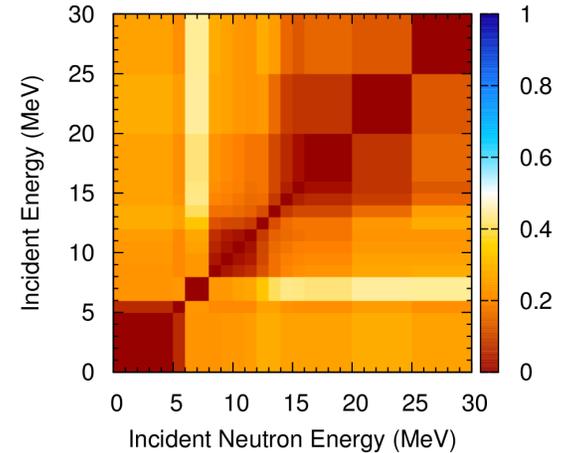
- Study from thermal to 30 MeV E_{inc}
- New data by CEA/LANL - Chatillon et al., BRC, 2014
- Take account of multi-chance fission and pre-equilibrium contributions

We recognized that a new LANL-LLNL experimental effort would be needed to reduce PFNS uncertainties – Chi-nu

But we are learning the challenges of identifying & reducing syst. errors

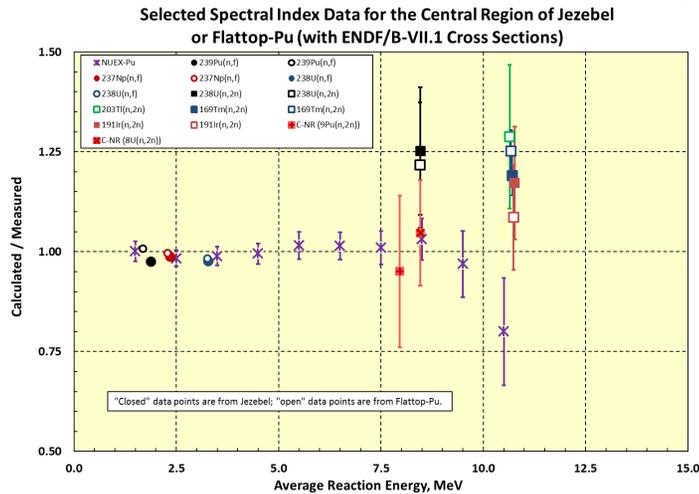
- Errors plagued previous experiments
- MCNP simulation is now playing a much larger role in guiding exp design

Mean of difference between correlations of different E_{inc}



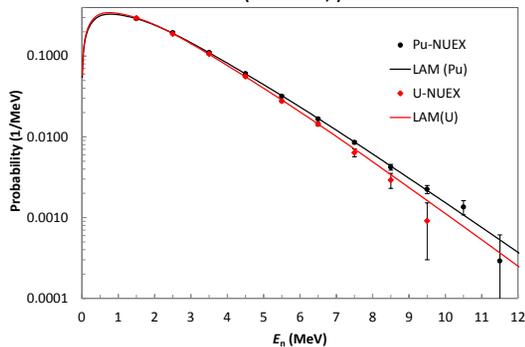
PFNS Solution will depend upon insights from Chi-nu & from various integral experiments

Activation – for the high-energy tail

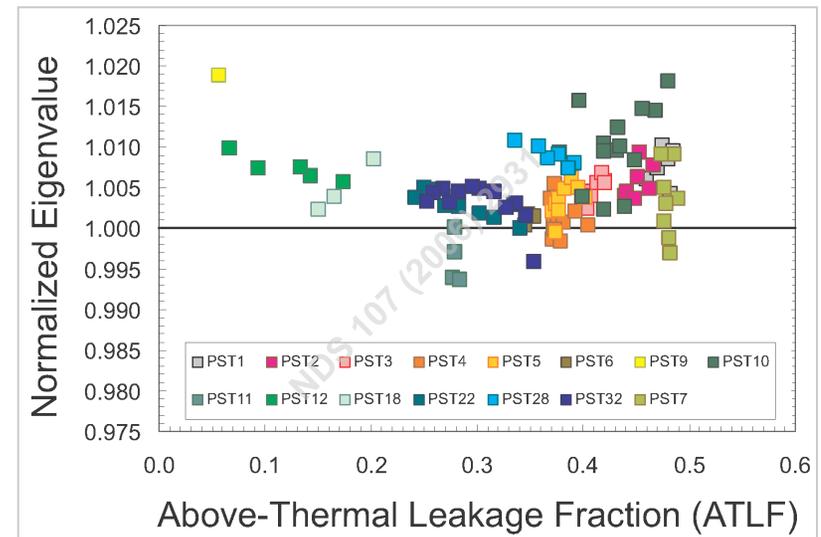


NUEX

Pu and U(1.5-MeV n,f) PFNS



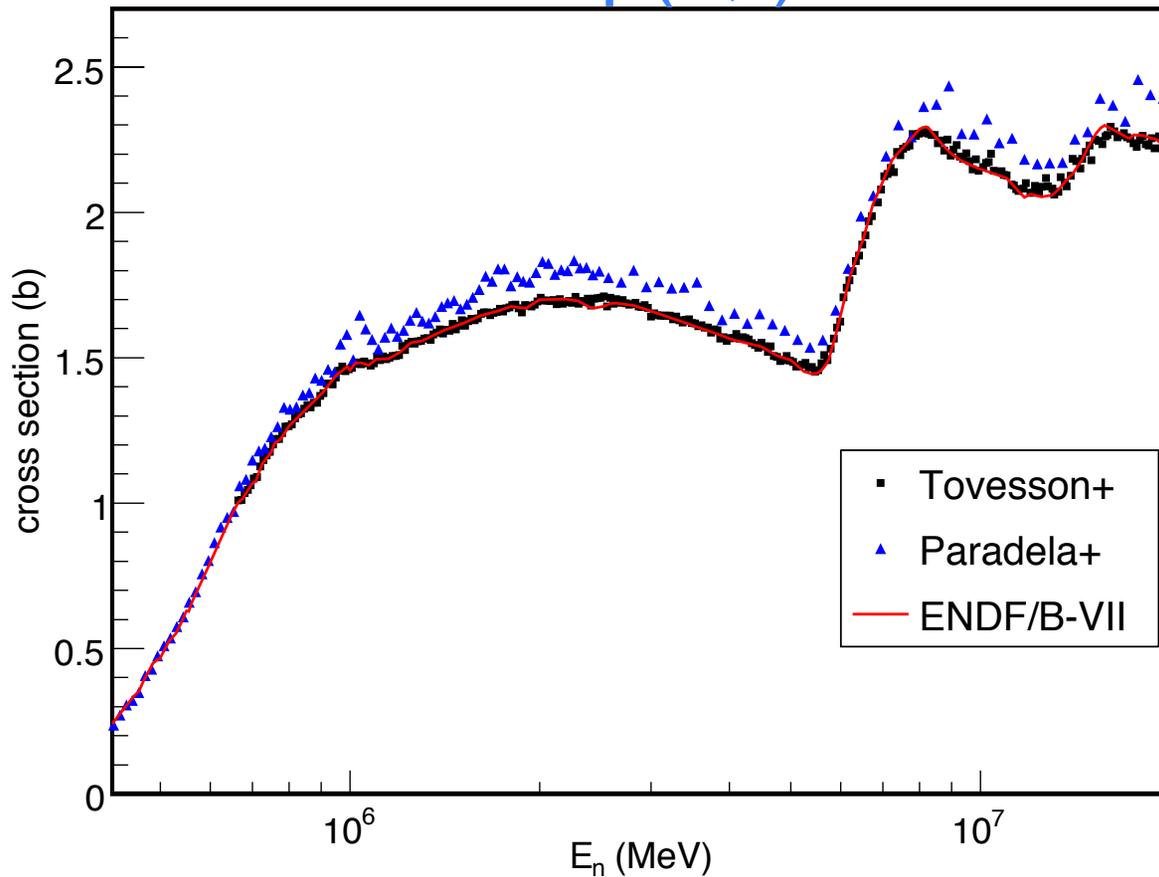
Criticality



At thermal there are fewer channels open. Increasingly likely that thermal PFNS will be slightly **harder** than ENDF/B-VII, which may be inconsistent with modifications at higher incident energies (which tend to be **softer**)

Example 3: Resolving Fission Cross Section Discrepancies will Require TPC

$^{237}\text{Np}(n,f)$



- LANL notes that semi-integral LANL fission spectral indices in crits support ENDF data
- CERN responds that puzzles regarding the simulation of the LANL-integral crit data for our Np-HEU sphere can be explained by their data

Example 3: Resolving Fission Cross Section Discrepancies will Require TPC

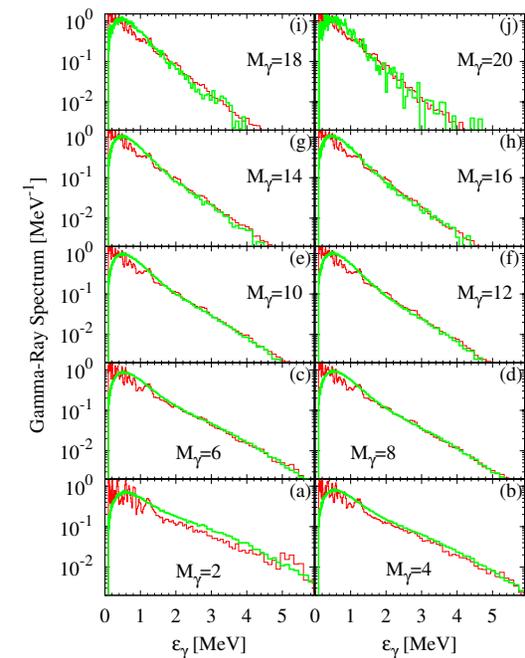
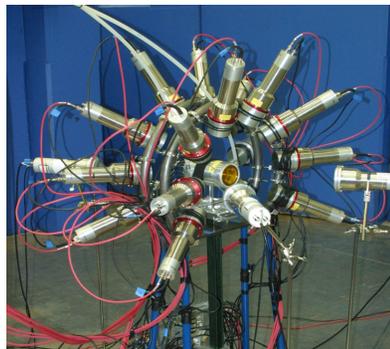
TABLE XXIX: Comparison of calculated spectra indices for ENDF/B-VII.0 with measured values in the center of various Los Alamos critical assemblies. $U238f/U235f$ refers to the ^{238}U fission rate divided by the ^{235}U fission rate, *etc.* Because ^{238}U and ^{237}Np are threshold fissioners, the spectral indices for these isotopes (in ratio to ^{235}U) measure the hardness of the neutron spectrum in the assembly Exp-A refers to experimental data as documented in the CSEWG Fast Reactor Benchmark Compilation, BNL 19302 (June 1973); Exp-B refers to the same measurements, but as reanalyzed by G. Hansen, one of the lead experimentalists, and transmitted to R. MacFarlane in 1984. The C/E ratios are based on the Hansen values where available.

Assembly	Quantity	$U238f/U235f$	$Np237f/U235f$	$U233f/U235f$	$Pu239f/U235f$
Godiva (HMF001)	Calc	0.15774	0.83002	1.56884	1.38252
	Exp-B	0.1643 ±0.0018	0.8516±0.012		1.4152 ± 0.014
	Exp-A	0.1642 ±0.0018	0.837 ±0.013	1.59±0.03	1.402±0.025
	Calc/Exp	C/E=0.9601	C/E=0.9747	C/E=0.9867	C/E=0.9769
Jezebel (PMF001)	Calc	0.20854	0.97162	1.55632	1.42453
	Exp-B	0.2133 ±0.0023	0.9835 ±0.014		1.4609 ± 0.013
	Exp-A	0.2137 ±0.0023	0.962 ±0.016	1.578 ±0.027	1.448 ±0.029
	Calc/Exp	C/E=0.9777	C/E=0.9879	C/E=0.9863	C/E=0.9751
Jezebel-23 (UMF001)	Calc	0.21065	0.98111		
	Exp-B	0.2131 ±0.0026	0.9970 ±0.015		
	Exp-A	0.2131 ±0.0023	0.977 ±0.016		
	Calc/Exp	C/E=0.9885	C/E=0.9841		
Flattop-25 (HMF028)	Calc	0.14443	0.77114	1.56725	1.35918
	Exp-B	0.1492 ±0.0016	0.7804 ±0.01	1.608 ±0.003	1.3847 ±0.012
	Exp-A	0.149 ±0.002	0.76 ±0.01	1.60 ±0.003	1.37 ±0.02
	Calc/Exp	C/E=0.9681	C/E=0.9881	C/E=0.9747	C/E=0.9816
Flattop-Pu (PMF006)	Calc	0.17703	0.85254		
	Exp-B	0.1799 ±0.002	0.8561 ±0.012		
	Exp-A	0.180 ±0.003	0.84 ±0.01		
	Calc/Exp	C/E=0.9840	C/E=0.9958		
Flattop-23 (UMF006)	Calc	0.18691	0.90801		
	Exp-B	0.1916 ±0.0021	0.9103 ±0.013		
	Exp-A	0.191 ±0.003	0.89 ±0.01		
	Calc/Exp	C/E=0.9755	C/E=0.9975		

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Future: In Addition to Synthesizing Cross Section & Integral Data, Future Evaluations Grounded in Full Correlations of Fission Data & Model Calculations

- **Ongoing NA-22 project: CGMF & FREYA in MCNP6**
 “Developing Accurate Simulations of **Correlated Data in Fission Events**”
- **Advances include:**
 - Predicting correlations and distributions of prompt neutrons and photons on an event-by-event basis (**CGMF**- Talou, Stetcu, Kawano; **FREYA**- Vogt, Randrup)
 - New and unique experimental data to benchmark model predictions
 - Univ. Michigan, **S.Pozzi** et al., **MCNPX-PoLiMi**
 - **DANCE**, **M.Jandel** et al.
 - Series of validation measurements at **NNSS/DAF**



Backup

Fission Never Ends ...

Plus Ultra : there is more beyond
(motto of the great scientific
pioneers of the 16th & 17th
Century)

Francis Bacon's *Novum Organum*
(1620): Straits of Gibraltar
flanked by the colossal pillars
of Hercules.

Inscription: Many shall pass too
and fro and knowledge shall
be increased



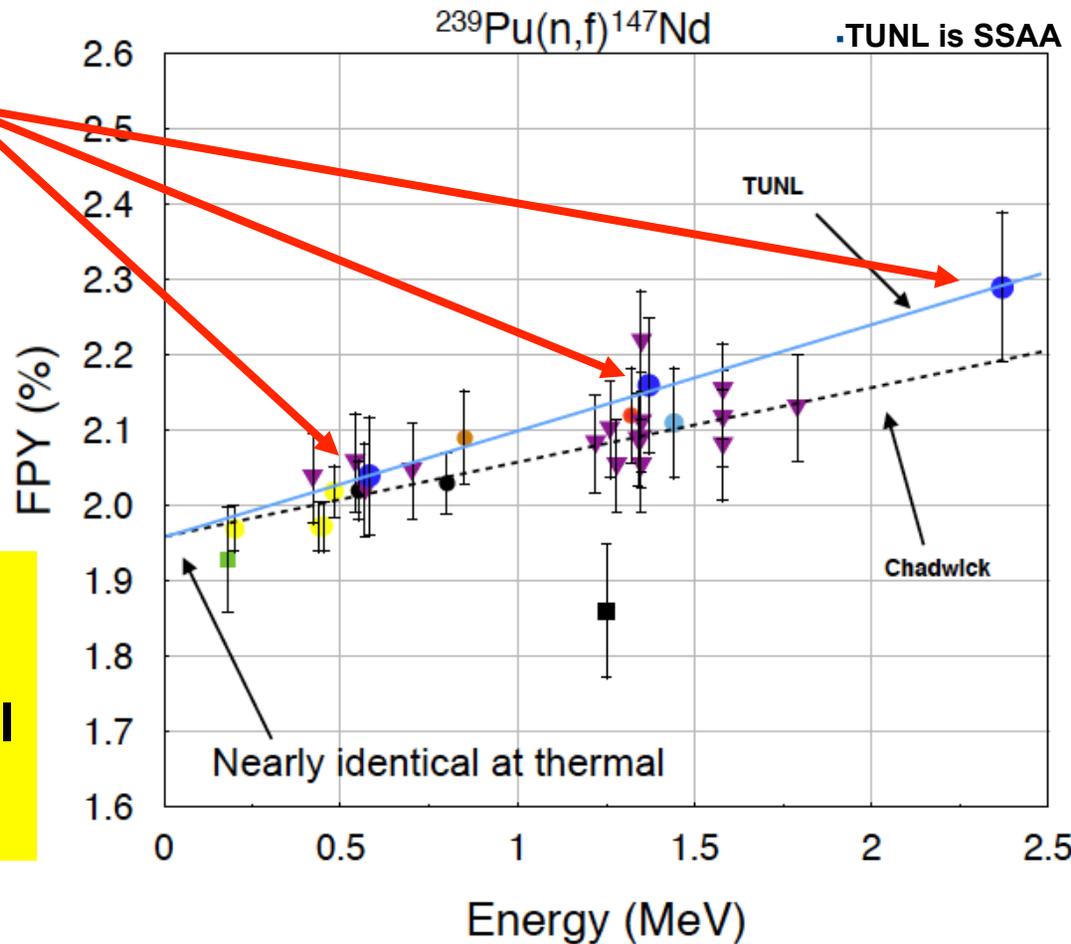
Resolution of Fission Yield Basis, for Plutonium. Confirmation of Energy-Dependence in Neodymium-147 Fission Product Yield

•LANL-LLNL-TUNL

•TUNL is SSAA Funded

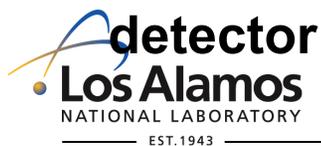


•New
TUNL
Data



- TUNL
- ▼ Selby
- Maeck
- Nethaway
- Lisman
- Rajagopalan
- Koch
- Gabeskiriya
- Laurec

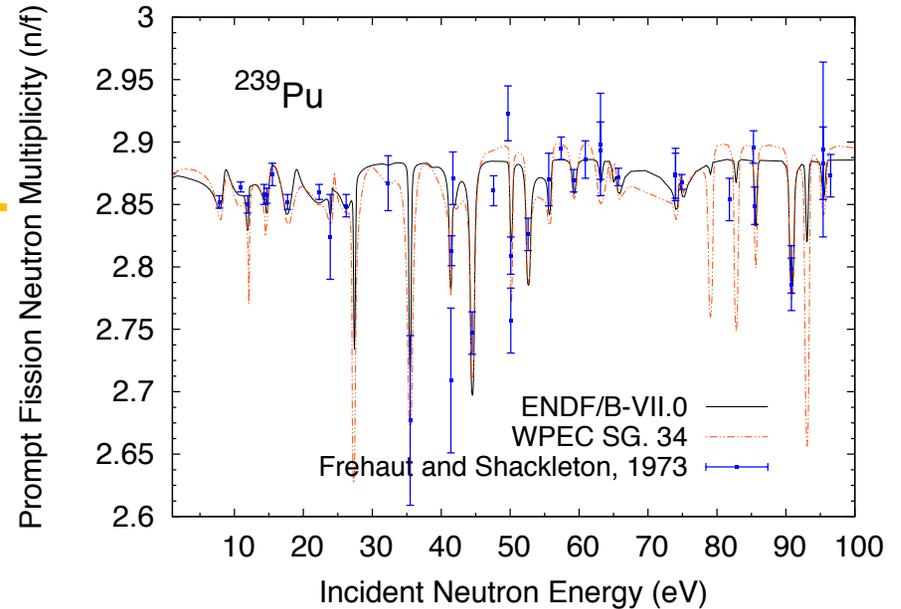
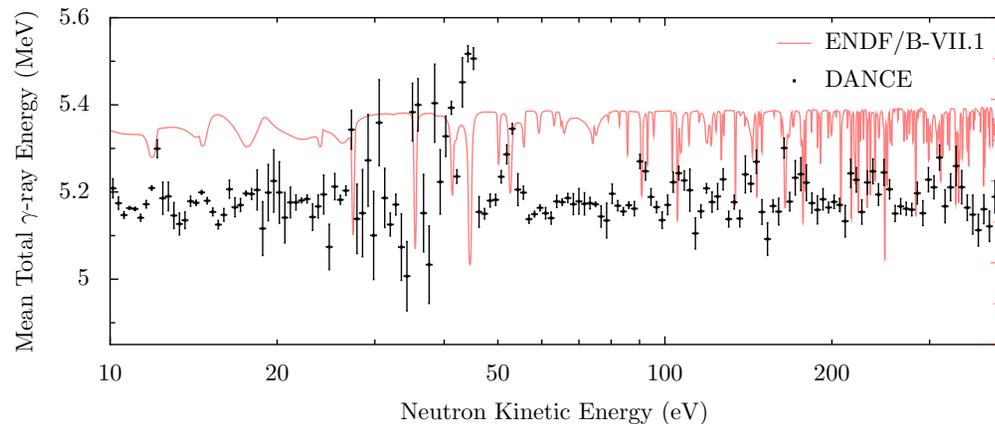
•Remaining open questions will be solved by the SPIDER



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The (n, γ f) process

- Fluctuations of $\langle v_p \rangle$ in RRR
- New DANCE measurements (Mosby, Couture), showing fluctuations of $\langle E_\gamma^{\text{tot}} \rangle$ in RRR



(n, γ f) would **increase** $\langle N_\gamma \rangle$ by ~ 1 , and reduce E^* available for prompt neutron emission by ~ 1 MeV, hence **reduce** $\langle v_p \rangle$

Early studies: J.E.Lynn, Phys. Lett. **18**, 31 (1965);
Stavinsky, V. and Shaker, M.O., Nucl. Phys. **62**, 667 (1965).

Fission Fragment Angular Distributions

- Original idea of **A. Bohr** (1959) following the experimental observation of strong anisotropies in fission fragment angular distributions

$$d\sigma_f(\theta) = \sum_J \sum_{M=-J}^J \sigma(JM) \sum_{K=0}^J \frac{\Gamma_f(JK)}{\Gamma(J)} \frac{2J+1}{4} \left(|D_{MK}^J(\theta)|^2 + |D_{M-K}^J(\theta)|^2 \right) \sin\theta d\theta$$

s-wave neutrons on even target: $W(KI) = \frac{1}{4}(2I+1) \left[|d_{1/2,K}^I(\theta)|^2 + |d_{-1/2,K}^I(\theta)|^2 \right]$

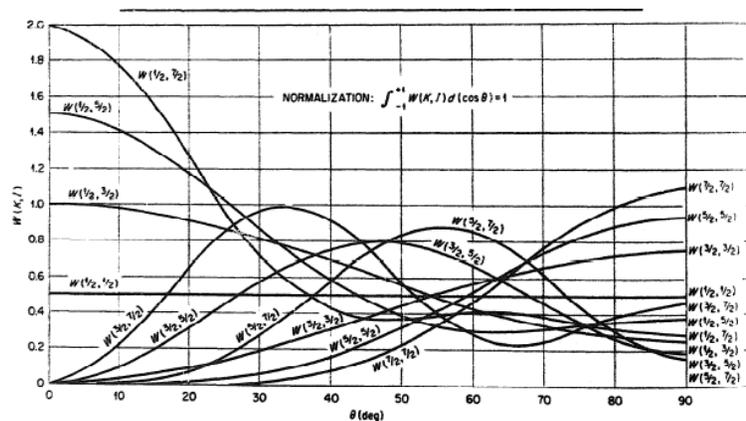
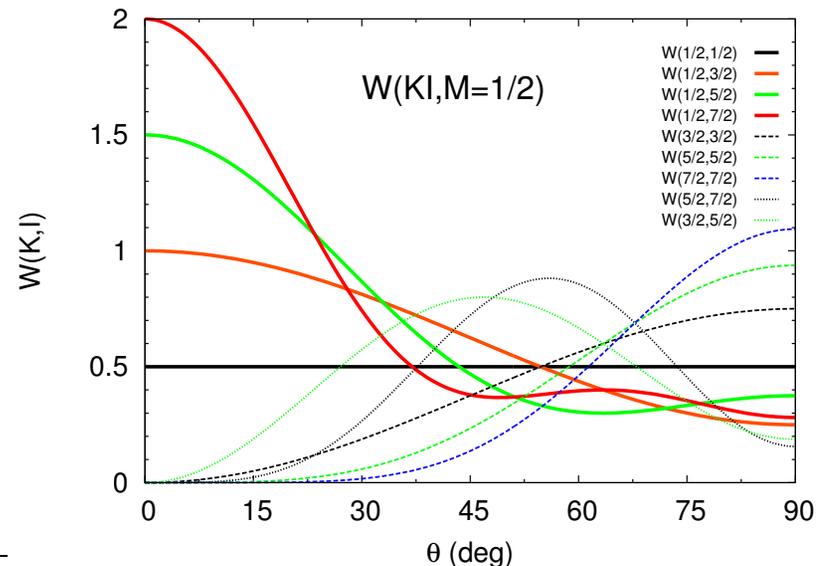


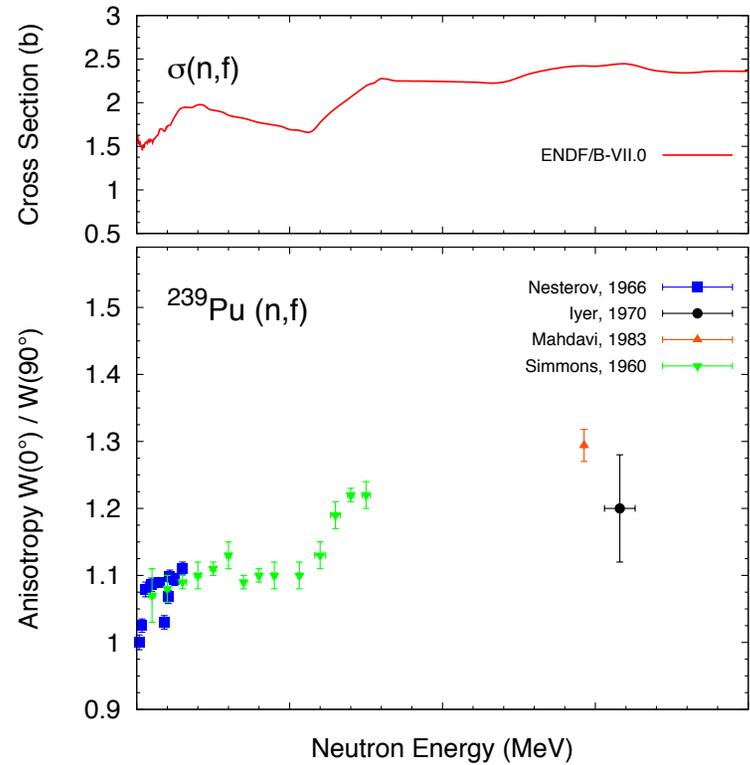
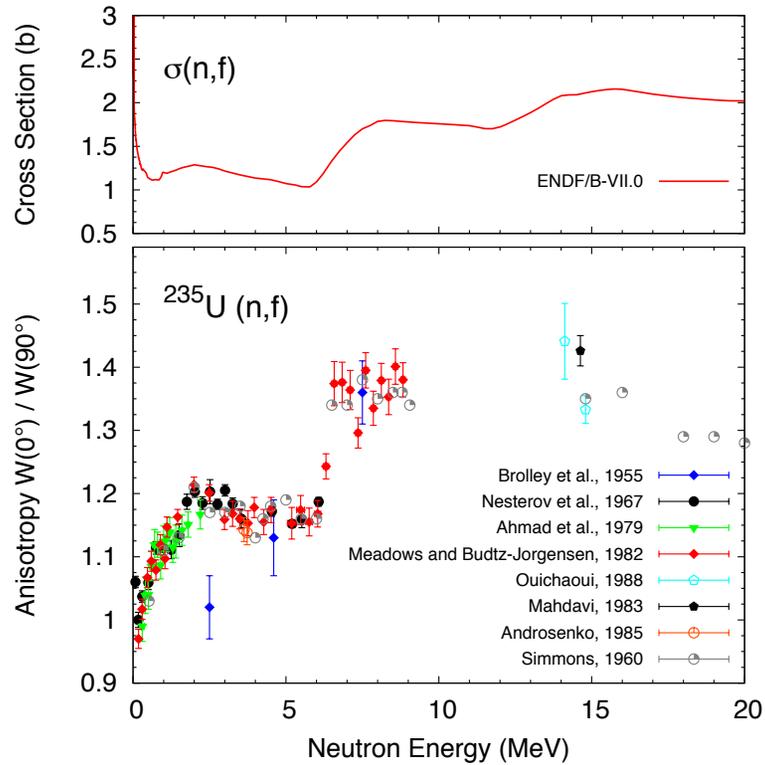
Fig. 6. Theoretical fission fragment angular distributions for fission through pure rotational states, $W(KI)$.

Lamphere, Nucl. Phys. **A38**, 661 (1962)



EST. 1943

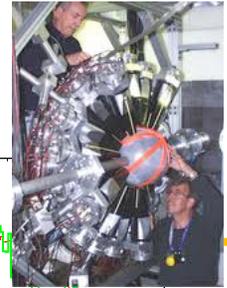
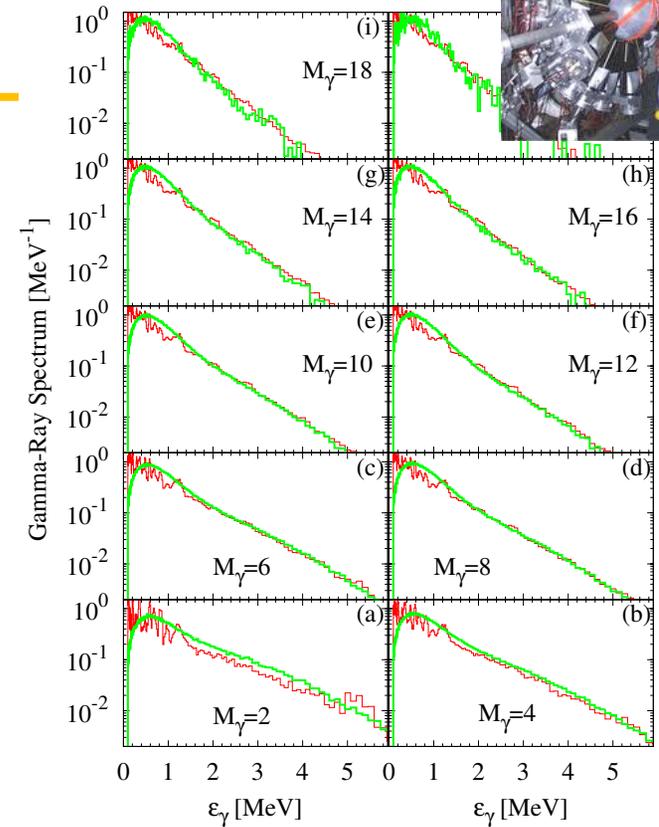
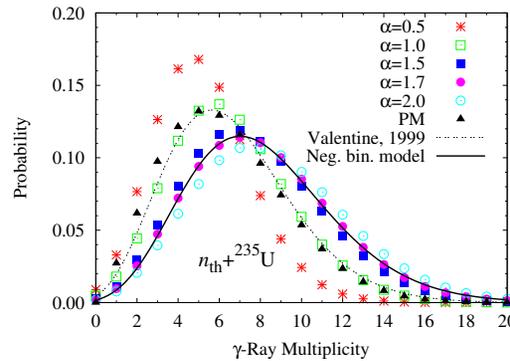
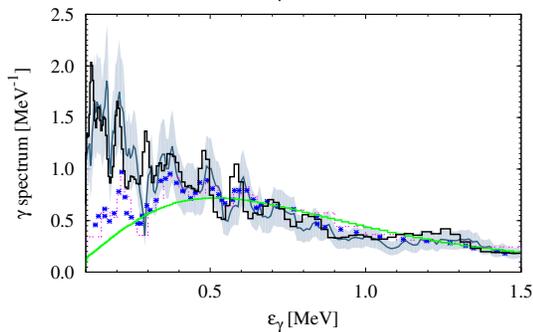
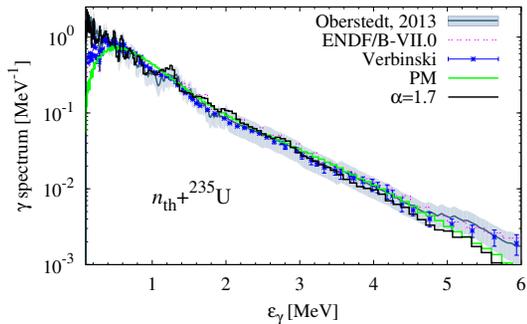
Incident-Energy Dependent Anisotropy



Ongoing experimental work at LANSCE, **V. Kleinrath**, **F. Tovesson**
 Also, talk by **L.S. Leong**

The Future is

- Monte Carlo Hauser-Feshbach code CGMF
- Stetcu, Talou, Kawano, Jandel, PRC 90, 024617 (2014)
- Ullmann et al., PRC 87, 044607 (2013)



Need for accurate pre-neutron emission fission fragment yields in mass, charge and TKE as a function of excitation energy!

(many talks/posters on this at FIESTA)

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